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ATLAS OF ZEOLITE STRUCTURE TYPES

by

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PREFACE

The steadily growing number of known zeolite structures and numerous requests which have been received for a previous survey of zeolite framework types has led to the present "Atlas of Zeolite Structure Types". The primary aim of the present compilation is to define and to supply a condensed characterization of the 38 currently established zeolite structure types. Apart from the stereopairs illustrating the framework structures the Atlas contains summaries of structural data as well as a Structure Type Index that includes all natural and synthetic materials which have been shown to be an isotype of a known zeolite structure type.

The present Atlas contains only reasonably well-established structures which have been at least partially refined. A number of zeolite structures included are by necessity based on powder data. A total of 38 structure types could, after critical assessment of the respective structure analysis, be included in this Atlas (compared to 27 in the previous survey by Meier and Olson, 1971).

Zeolites do not comprise an easily definable family of crystalline aluminosilicates. The inclusion or exclusion of borderline cases was decided on the basis of criteria used at recent International Conferences on zeolites.

We wish to acknowledge the use of the stereographic computer plotting program ORTEP, written by Dr. Carroll K. Johnson (Oak Ridge National Laboratory). A listing of the ORTEP input used to generate the stereopairs in this Atlas has been deposited as document number NAPS-03331. (Order from ASIS/NAPS, Microfiche Publications, P.O. Box 3513, Grand Central Station, New York, N.Y. 10017). Information obtained by private communication in addition to the published data has in several instances been used in the preparation of the Atlas. Such use is indicated in the References and we gratefully acknowledge this help. We also wish to thank our colleagues of the IZA Structure Commission for critically

Explanatory Notes

Probably the simplest way of illustrating zeolite structures is by means of skeletal models or diagrams showing the 4-connected nets formed by the tetrahedral atoms in the various aluminosilicate frameworks. The known zeolite framework types are presented in this Atlas by means of stereographic drawings of this kind. In general, the viewing direction (which is stated in each case) has been chosen in such a way that the main channels are clearly visible. The unit cell has also been outlined whenever possible and provided that no change in symmetry is effecting the cell edges have been encountered. The positions of ... atoms (T = Si,Al) are those of the points or vertices of the net and the T-O-T bridges are represented by straight lines. The positions of the O-atoms are only approximately displayed in these diagrams since the T-O-T angles are typically around $140-150°$. The idealization makes it easier to visualize the topology and basic features of zeolite framework structures which in many instances are relatively complex.

STRUCTURE TYPE

Structural classifications of zeolites are primarily based on the topology of the frameworks. Zeolite species which do not differ with respect to the framework topology are called isotypic, i.e. they represent the same structure type irrespective of composition, distribution of the different T-atoms, cell dimensions, and symmetry. A mnemonic code consisting of 3 capital letters has been adopted for each structure type following the recommendations by IUPAC on zeolite nomenclature[1].

1) "Chemical Nomenclature, and Formulation of Compositions, of Synthetic and Natural Zeolites", prepared by a special IUPAC Commission under the chairmanship of R. M. Barrer. IUPAC yellow booklet, 1978.

Structure type codes are generally derived from the names of the type species (see below) and do not include numbers and characters other than capital roman letters. Since structural criteria alone do not provide an unambiguous numbering scheme, and to facilitate later additions and simple indexing, the various structure types in this Atlas have been arranged in alphabetical order according to the structure type code. For each structure type the information given in bold type codes the full type name, the maximum topological symmetry (i.e. the maximum possible space group) and a listing of the topologically distinct T-atoms, their number per unit cell, as well as the maximum point symmetry of the respective T-sites (in square parentheses).

Secondary Building Units (SBU)

Zeolite frameworks can be thought to consist of finite or infinite (i.e. chain- or layer-like) component units. The finite units containing up to 16 T-atoms, which have been found to occur in framework silicates, are shown in Figure 1. These secondary building units[1] are derived assuming the entire framework is made up of one type of SBU only[2]. A unit cell invariably contains an integral number of SBU. Many of the frameworks can be built from several different SBU. In these cases the SBU listed in the first place is the one which occurs most frequently in related structures.

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1) The primary building units being the single TO_4 tetrahedra.
2) There is evidence, however, that some zeolite frameworks consist of two component units, such as 4-membered rings of silica tetrahedra which are linked to each other through single AlO_4 tetrahedra as in the case of laumontite and (possibly) analcime.
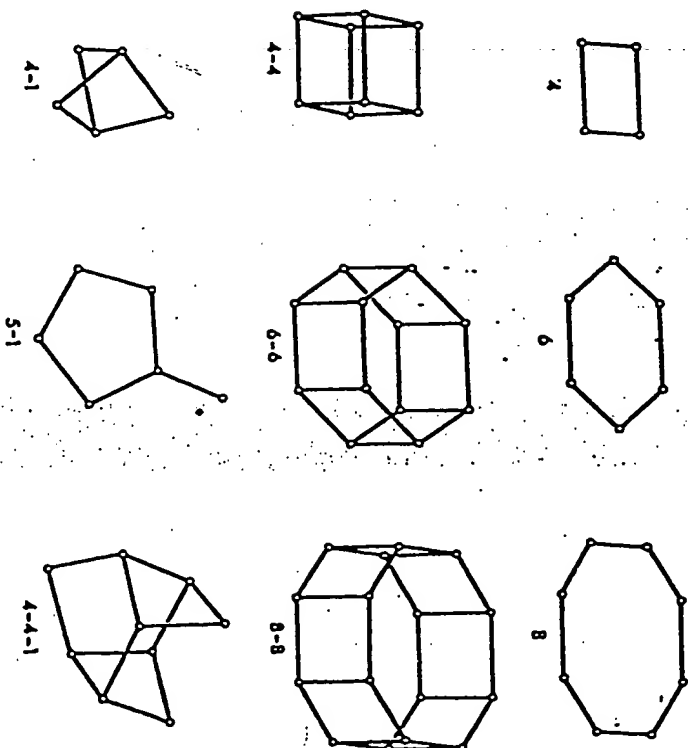
Figure 1

Framework Density (FD)

This is defined as the number of T-atoms per 1000 $Å^3$. For most framework structures values of at least 20 T/1000 $Å^3$ are generally obtained while for zeolites the observed values range from about for structures with the largest pore volume to around 20. The FD is obviously related to the pore volume but does not reflect the size of the pore openings. For some non-rigid zeolite structure types the FD values can vary appreciably. In these cases (such as gismondine) values are given for the type species and the framework in the most expanded state. The flexibility of the framework structure is to some extent displayed by the possible variation of the FD.

orthand notation has been adopted for the description of the chan- In the various frameworks. Each system of equivalent channels been characterized by ne channel direction (relative to the axes of the type structure) ne number of either T- or O-atoms (underlined number) forming ne smallest rings of the channels, and he crystallographic free diameters of the channels.

free diameter values are based on the atomic coordinates of the species in the hydrated state and an oxygen radius of 1.35 A. minimum and maximum values are given for non-circular apertures. many instances the corresponding interatomic distance vectors are approximately co-planar, and closer inspection of the diagrams ld give some information on this in the first instance. It should be noted that crystallographic free diameters depend on the state composition of the zeolite, and can differ appreciably for various ypic species, particularly in the case of non-rigid frameworks.

number of asterisks in the notation used indicates whether the chan- system is one-, two- or three-dimensional. Only those apertures taken into account which are more open than regular six ed rings. In most cases these smaller openings simply form dows (rather than channels) connecting larger cavities. Interconnect- channel systems are separated by a double arrow (⟷). A ver- bar (|) means that there is no direct access from one channel tem to the other.

selected examples in Table 1 illustrate the various possibilities the use of the notation. Cancrinite is characterized by a one- ensional system of channels parallel to [001] or c with circular ring apertures. In offretite the main channels form a similar system are interconnected by channels made of 8-rings giving rise to a

3-dimensional channel sy   . The channel system in m   hite is es- sentially 2-dimensional, the 12-ring apertures of the mai.. channels being somewhat elliptical. Paulingite is an example of a framework type containing two independent sets of 3-dimensional channel systems which are displaced against each other. (<100> means there are chan- nels parallel to all crystallographically equivalent axes of the cubic structure, i.e. along x, y and z). In gismondine the channels parallel to [100] together with those parallel to [010] give rise to a 3- dimensional channel system which can be pictured as an array of partially overlapping tubes.

Table 1: EXAMPLES ILLUSTRATING THE NOTATION FOR THE CRYS- TALLOGRAPHIC CHARACTERIZATION OF THE CHANNEL

|		
Cancrinite	[001] 12 6.2 *	
Offretite	[001] 12 6.4 * ⟷ ⊥ [001] 8 3.6 x 5.2 **	
Mordenite	[001] 12 6.7 x 7.0 * ⟷ [010] 8 2.9 x 5.7 *	
Paulingite	<100> 8 3.9 *** | <100> 8 3.9 ***	
Gismondine	{[100] 8 3.1 x 4.4 ⟷ [010] 8 2.8 x 4.9} ***	

Fault Planes (FP)

Likely FP are listed for each structure type. The existence of FP means that layer-like segments of the framework can be stacked in more than one way, giving rise to polytypism. A number of related structures (polytypes) can be readily postulated on this basis. FP also serve as an indication of possible stacking faults which may affect the critical channel dimensions.

Type Species and References

The type species stated in the data section is the species used to establish the structure type. In the majority of cases these have been natural zeolites providing single crystal data. The composition expressed in terms of cell contents has in many cases been idealized inasmuch as compositional data give average unit cell contents which frequently correspond to fractional numbers of atoms. Isotypic species are very common and have been listed in the Index.
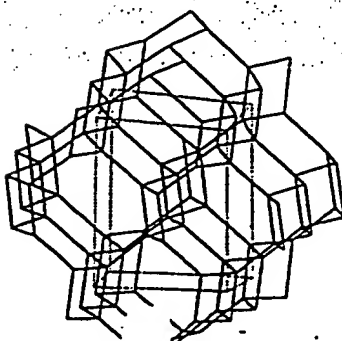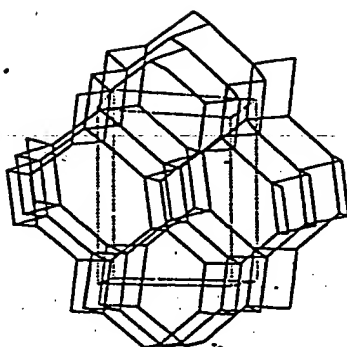
Li-A(BW)   Imam   8 T[m

viewed along [001]

Secondary building units: single 4-rings (single 6- or 8-rings)

Framework density: 19.0 T/1000 A³

Channels: [001] 8 3.6 x 4.0 *
(010), (011)

Fault planes: (010), (011)

Type species: synthetic zeolite Li-A (Barrer + White)
$Li_4Al_4Si_4O_{16}$ · 4 H_2O
orthorhombic, Pna2₁, a=10.3 b=8.2 c=5.0 Å

References:
¹) I.S. Kerr (1974)

Structure Type Index

Type species are marked by an asterisk. To make the index as informative as possible all reported species and designations have been included in this section, provided the structure type assignment appears reasonably well established. Even a number of occasionally used but discredited names of mineral species have been included in this index for the afore-mentioned reason. Moreover, the inclusion of a synthetic species designation in this index must not be interpreted to mean that the designation has been formally recognized or generally accepted but merely that the material has one of the established structure types. References have been restricted to those considered necessary to identify the species. For unreferenced minerals, see Strunz (1977).

*	Afghanite	AFG	G. T. Wadinger, E. J. Rosinski, and C. J. Plank (1968)
	ALPHA	LTA	
	A, Na-A	LTA	D. W. Breck, W. G. Eversole, R. M. Milton, T. B. Reed and T. L. Thomas (1956)
*	Analcime	ANA	
—	Analcite	ANA	
	B	GIS	R. M. Milton (1961)
	Ba-G	LTL	R. M. Barrer and D. J. Marshall (1964)
	Ba-P	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
	Ba-Q	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
	Barrerite	STI	E. Passaglia and D. Pongiluppi (1975)
	Basic cancrinite	CAN	R. M. Barrer and E. A. D. White (1952)
	Basic sodalite	SOD	R. M. Barrer and E. A. D. White (1952)
*	Bikitaite	BIK	
*	Brewsterite	BRE	

Mineral	Code	Reference
Ca-D	ANA	L. L. Ames and L. B. Sand (1958)
Cancrinite	CAN	I. Wyart and Michel-Lévy (1949)
Cancrinite hydrate	CAN	
Chabazite	CHA	A. Alberti (1975)
Clinoptilolite	HEU	
CsAlSiO₄	ABW	S. J. Chung and Th. Hahn (1972)
Cs-D	CHA	D. W. Beck and N. A. Acara (1960)
Dachiardite	DAC	
Danalite	SOD	
Desmine	STI	
Edingtonite	EDI	
Epidesmine	STI	
Epistilbite	EPI	
Erionite	ERI	
Faujasite	FAU	
Ferrierite	FER	G. P. L. Walker (1962)
Garronite	GIS	
Gismondine	GIS	
Gmelinite	GME	
●ardite	THO	W. Borchert and J. Keidel (1947)
Harmotome	PHI	R. M. Barrer and D. J. Marshall (1964)
Herschelite	CHA	D. McConnell (1964)
Heulandite	HEU	
Hydroxysodalite	SOD	R. M. Barrer and J. W. Baynham (1956)
(K, Ba) -G	LTL	
Keholte	ANA	R. M. Barrer and J. W. Baynham (1956)
K-F	EDI	
K-M	MER	R. M. Barrer and J. W. Baynham (1956)
Laubanite	NAT	
Laumontite	LAU	
Leucite	ANA	

Mineral	Code	Reference
Leonhardite	LAU	C. T. Amirov, V. V. Ilyukhin and N. V. Belov (1967)
* Levyne	LEV	
Levynite	LEV	
* Li-A	ABW	R. M. Barrer and E. A. D. White (1951)
* Linde A	LTA	D. W. Breck, W. G. Eversole, R. M. Milton, T. B. Reed and T. L. Thomas (1956)
Linde B	GIS	R. M. Milton (1961)
Linde D	CHA	D. W. Breck and N. A. Acara (1960)
* Linde L	LTL	D. W. Breck and E. M. Flanigen (1960)
Linde R	CHA	R. M. Milton (1960)
Linde T	OFF-ERI	D. W. Breck and N. A. Acara (1960)
Linde W	MER	R. M. Milton (1961)
Linde X	FAU	R. M. Milton (1959)
Linde Y	FAU	D. W. Breck (1964)
* Liottite	LIO	
* Losod	LOS	W. Sieber and W. M. Meier (1974)
* Mazzite	MAZ	
* Merlinoite	MER	
* Mordenite	MOR	
N-A	LTA	R. M. Barrer and P. J. Denny (1961)
Na-B	ANA	R. M. Barrer and E. A. D. W. .195
Na-D	MOR	R. M. Barrer and E. A. D. White (19
Na-P1	GIS	R. M. Barrer, F. W. Bultitude and I. S. Kerr (1959)
Na-P2	GIS	R. M. Barrer, F. W. Bultitude and I. S. Kerr (1959)
* Natrolite	NAT	
Nosean	SOD	
O	OFF	
* Offretite	OFF	R. Alello and R. M. Barrer (1970)
Omega	MAZ	
* Paulingite	PAU	E. M. Flanigen (1968)

	Name	Code	Reference
	P-[Cl.]	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
	Pc, Pt	PHI	A. M. Taylor and R. W. Roy (1964)
*	Phillipsite	GIS	
	P-L	LTL	E. M. Flanigen and R. W. Grose (1971)
	P, Na-P	GIS	R. M. Barrer, J. W. Baynham, F. W. Bultitude, and W. M. Meier (1959)
●	Pollucite	ANA	
	Ptilolite	MOR	
	Q-[Br]	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
	R	CHA	R. M. Milton (1960)
	RbAlSiO$_4$	ABW	S. J. Chung and Th. Hahn (1972)
*	Rho	RHO	H. E. Robson, D. P. Shoemaker, R. A. Ogilvie and P. C. Manor (1973)
	Scolecite	NAT	
	S, Na-S	GME	R. M. Barrer, J. W. Baynham, F. W. Bultitude and W. M. Meier (1959)
	Sr-Q	YUG	R. M. Barrer and D. J. Marshall (1964)
●	Sodalite hydrate	FER	R. M. Barrer and D. J. Marshall (1964)
	-D	SOD	J. Wyart and M. Michel-Lévy (1949)
*	Sodalite	SOD	
*	Stilbite	STI	
*	Stellerite	STI	
τ	T	OFF-ERI	D. W. Breck and N. A. Acara (1960)
	Tetracalcium trialuminate	SOD	V. I. Ponomarev, D. M. Kheiker and N. V. Belov (1970)
*	Thomsonite	THO	R. Aiello and R. M. Barrer (1970)
*	TMA-E	EAB	H. Sorensen (1963)
	Tugtupite	SOD	
	Ultramarine	SOD	
	Viselte	ANA	J. Melon (1942)

	Name	Code	Reference
	W	MER	R. M. Milton (1961)
	Wairakite	ANA	A. Steiner (1955)
*	Wellsite	PHI	P. Cerny, R. Rinaldi and R. C. ...dam (1977)
	X	FAU	R. M. Milton (1959)
	Y	FAU	D. W. Breck (1964)
*	Yugawaralite	YUG	
	Zeolon	MOR	
	Zh	SOD	S. P. Zhdanov and N. N. Buntar []
	ZK-4	LTA	G. T. Kerr (1966)
*	ZK-5	KFI	G. T. Kerr (1963)
	ZK-19	PHI	G. H. Kühl (1969)
	ZK-20	LEV	G. T. Kerr (1969)
	ZK-21	LTA	G. H. Kühl (1967, 1971)
	ZK-22	LTA	G. H. Kühl (1967, 1971)
	ZSM-4	MAZ	J. Ciric (1967)
*	ZSM-5 ')	MFI	R. J. Argauer and G. R. Landolt (1972)
*	ZSM-11	MEL	P. Chu (1973)

') Recently, E. M. Flanigen et al (1978) reported a silica polymorph having the MFI structure type.